Quantum phase transition and underscreened Kondo effect in electron transport through parallel double quantum dots

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We investigate electronic transport through parallel double quantum dot(DQD) system with strong on-site Coulomb interaction and capacitive interdot coupling. By applying numerical renormalization group(NRG) method, the ground state of the system and the transmission probability at zero temperature have been obtained. For a system of quantum dots with degenerate energy levels and small interdot tunnel coupling, the spin correlations between the DQDs is ferromagnetic, and the ground state of the system is a spin 1 triplet state. The linear conductance will reach the unitary limit ($2e^2/h$) due to the underscreened Kondo effect at low temperature. As the interdot tunnel coupling increases, there is a quantum phase transition from ferromagnetic to anti-ferromagnetic spin correlation in DQDs and the linear conductance is strongly suppressed.

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I. INTRODUCTION

In recent years considerable research attention has been paid to electron transport through double quantum dot(DQD)systems[1], which are an artificial small quantum systems can be readily controlled by external gate voltage and also exhibit a variety of interesting strongly correlated electron behaviors. Basically, there are two different experimental realizations of DQD system: DQDs connected in serial[2] or in parallel configurations[3]. Electron transport through both configurations have been studied in experiments, the molecular states of the double dots and also the competition between Kondo effect and the RKKY interaction have been observed[2, 3].

The theoretical studies on electron transport through DQDs are largely devoted to the system in the Kondo regime. For DQDs connected in serial, the antiferromagnetic correlations between two single-level coupled QDs is in competition with Kondo correlations between the QDs and the electrons in the leads, therefore it gives rise to rich ground state physical properties at zero temperature[4, 5, 6, 7]. For DQDs with large capacitive coupling, the simultaneous appearance of the Kondo effect in the spin and charge sectors results in an SU(4) Fermi liquid ground state[8]. By increasing interdot capacitive coupling, a quantum phase transition of Kosterlitz-Thouless type to a non-Fermi-liquid state with anomalous transport properties is predicted[9]. Martins et al argued that ferromagnetic state cannot be realized in two single-level QDs connected in serial, but they predicts that FM state can be developed in two double-level QDs[10]. For the DQD system in parallel configuration, the physical properties can be quite different, since the interference effect will play an important role in its transport properties. The Fano effect for electron transport through bonding and antibonding channels in DQDs system has been studied[11, 12, 13].

Due to the strong correlation of electrons in the QDs, it is a non-trivial problem to treat those systems theoretically. It is well known that Wilson's numerical renormalization group[14, 15, 16, 17] method is a nonperturbative approach to quantum impurity problem, which can take into account the on-site Coulomb repulsion and the spin exchange interaction between the electrons in DQDs exactly, in contrast to the slave boson mean field theory or the equation of motion method within Hartree-Fock approximation. The NRG method have already been applied to investigate a lot of problems in the electron transport through QD systems. For instance, DQDs connected in serial[18], the quantum phase transition in multilevel QD[19], Kondo effect in coupled DQDs with RKKY interaction in external magnetic field[20], the side coupled DQD system[21, 22] and quantum phase transitions in parallel quantum QDs [23] etc. However, in our opinion the consequences of the interplay of Fano resonance and the Kondo effect on electron conductance through DQDs in parallel still haven't been well elucidated. In this paper we will investigate the electron transport properties for the DQDs in parallel configuration by using the NRG method. We will show that for DQDs without interdot tunneling, the underscreen Kondo effect plays an essential role in the conductance. The linear conductance, spin correlation, and local density of state in this system are obtained.

II. THE MODEL HAMILTONIAN AND THE NRG APPROACH

Electron transport through parallel-coupled DQDs with interdot tunneling, on-site Coulomb interaction and capacitive interdot coupling can be described by the following Anderson impurity model:

$$H = \sum_{k\eta\sigma} \epsilon_{k\eta} c^\dagger_{k\eta\sigma} c_{k\eta\sigma} + \sum_{i\sigma} \epsilon_i d^\dagger_{i\sigma} d_{i\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow} + V n_1 n_2$$

$$+ \ t_c \sum_{\sigma}(d^{\dagger}_{1\sigma}d_{2\sigma} + d^{\dagger}_{2\sigma}d_{1\sigma}) + \sum_{k\eta\sigma i}(v_{\eta i}d^{\dagger}_{i\sigma}c_{k\eta\sigma} + H.c.) \ , \quad (1)$$

where $c_{k\eta\sigma}(c^{\dagger}_{k\eta\sigma})$ denote annihilation(creation) operators for electrons in the leads($\eta = L, R$), and $d_{i\sigma}(d^{\dagger}_{i\sigma})$ those of the single level state in the i-th dot($i = 1, 2$). $n_{i\sigma}$ denotes the electron number operator with spin index σ in the i-th dot, and $n_i = \sum_{\sigma} n_{i\sigma}$. U is the intra-dot Coulomb interaction between electrons, V is the interdot capacitive coupling. t_c is the interdot tunnel coupling, and $v_{\eta i}$ is the tunnel matrix element between lead η and dot i. It should be noted that an interdot magnetic exchange term J is not explicitly included in this Hamiltonian since it is not an independent parameter but a function of the interdot tunneling($J \sim t_c^2/U$). We consider the symmetric coupling case with $\Gamma^L_i = \Gamma^R_i = \Gamma_i$, where $\Gamma^{\eta}_i = 2\pi\sum_k |v_{\eta i}|^2\delta(\omega - \epsilon_{k\eta\sigma})$ is the hybridization strength between the i-th dot and the lead η.

In order to access the low-energy physics of this DQD system, we adopt the Wilson's NRG approach. By symmetric combination of the lead orbitals, the Hamiltonian in eq.(1) can be mapped to single-channel two-impurity Anderson model. Because the anti-symmetric combination of lead orbitals are totally decoupled with the QDs, they can be neglected in the Hamiltonian. Following the standard NRG method, one defines a series of rescaled Hamiltonian H_N as following

$$\begin{aligned} H_N \ &= \ \Lambda^{(N-1)/2}[\sum_{\sigma,n=0}^{N-1}\Lambda^{-n/2}\xi_n(f^{\dagger}_{n\sigma}f_{n+1\sigma} + f^{\dagger}_{n+1\sigma}f_{n\sigma}) \\ &+ \ \sum_{i\sigma}(\tilde{\epsilon}_i + \frac{1}{2}\tilde{U})d^{\dagger}_{i\sigma}d_{i\sigma} + \frac{1}{2}\tilde{U}\sum_i(n_i - 1)^2 + \tilde{V}n_1n_2 \\ &+ \ \tilde{t}_c\sum_{\sigma}(d^{\dagger}_{1\sigma}d_{2\sigma} + d^{\dagger}_{2\sigma}d_{1\sigma}) + \sum_{i\sigma}\tilde{\Gamma}_i^{1/2}(f^{\dagger}_{0\sigma}d_{i\sigma} + d^{\dagger}_{i\sigma}f_{0\sigma})] \ , \end{aligned} \quad (2)$$

where the discretization parameter $\Lambda = 1.5$, and $\xi_n \approx 1$[17]. The other parameters $\tilde{\epsilon}_i = \frac{2}{1+\Lambda^{-1}}\frac{\epsilon_i}{D}$, $\tilde{U} = \frac{2}{1+\Lambda^{-1}}\frac{U}{D}$,$\tilde{V} = \frac{2}{1+\Lambda^{-1}}\frac{V}{D}$, $\tilde{t}_c = \frac{2}{1+\Lambda^{-1}}\frac{t_c}{D}$ and $\tilde{\Gamma}_i = (\frac{2}{1+\Lambda^{-1}})^2\frac{\Gamma_i}{\pi D}$, with D being the bandwidth of electrons in the leads. The above one dimensional lattice model is iteratively diagonalized by using the recursion relation

$$H_{N+1} = \Lambda^{1/2}H_N + \xi_n\sum_{\sigma}(f^{\dagger}_{N\sigma}f_{N+1\sigma} + f^{\dagger}_{N+1\sigma}f_{N\sigma}) \ . \quad (3)$$

The basis set in each iteration step is truncated by retaining only those states with low-lying energies. In our numerical calculation, we keep totally 600 low-lying energy states in each step without counting the S_z degeneracy.

The current formula through the DQDs is given by the generalized Landauer formula[24]

$$I = \frac{e}{h}\sum_{\sigma}\int d\omega[n_L(\omega) - n_R(\omega)]T(\omega) \ , \quad (4)$$

where the transmission probability $T(\omega) = -Tr[\hat{\Gamma}Im[\hat{G}^r(\omega)]]$, with $\hat{\Gamma} = \hat{\Gamma}^L = \hat{\Gamma}^R = \begin{pmatrix} \Gamma_1 & \sqrt{\Gamma_1\Gamma_2} \\ \sqrt{\Gamma_1\Gamma_2} & \Gamma_2 \end{pmatrix}$. The retarded/advanced Green's functions(GF) $\hat{G}^{r/a}(\omega)$ have 2×2 matrix structures, which account for the double dot structure of the system. The matrix elements of the retarded GF are defined in time space as $G^r_{ij}(t - t') = -i\theta(t - t') < \{d_{i\sigma}(t), d^{+}_{j\sigma}(t')\} >$. Therefore, the transmission probability $T(\omega)$ can be obtained by calculating the imaginary parts of the GF of DQDs or the spectral density $\rho_{ij}(\omega) = -\frac{1}{\pi}ImG^r_{ij}(\omega)$. Then, the linear conductance at the absolute zero temperature can be given by taking the zero frequency limit of the transmission probability $G = \frac{dI}{dV}|_{V=0} = \frac{2e^2}{h}T(\omega = 0)$. One advantage of the NRG is accurate determination of the low-energy spectral density of the quantum impurity models. By a standard procedure in NRG [17], the spectral density at zero temperature can be calculated according to the following formula

$$\begin{aligned} \rho_{ij}(\omega) \ &= \ \frac{1}{Z(0)}\sum_{\lambda}M^i_{0,\lambda}(M^j_{0,\lambda})^*\delta(\omega - (E_\lambda - E_0)) \\ &+ \ \frac{1}{Z(0)}\sum_{\lambda}M^i_{\lambda,0}(M^j_{\lambda,0})^*\delta(\omega + (E_\lambda - E_0)) \end{aligned} \quad (5)$$

where the matrix element $M^i_{\lambda,0} =< \lambda|d_{i\sigma}|0 >$, with $|0 >$ and $|\lambda >$ being the ground state and exited eigenstate of the impurity model Hamiltonian, respectively.

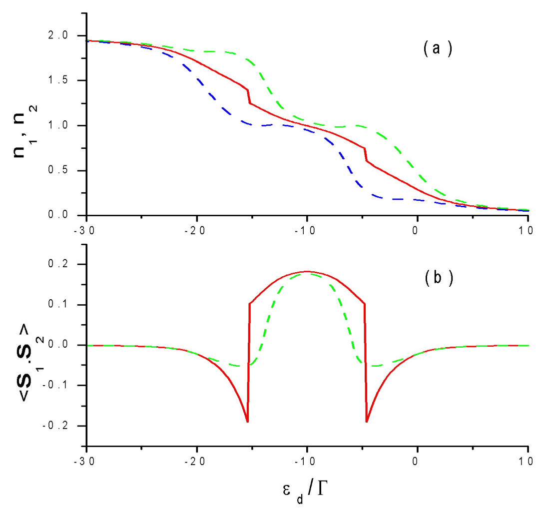

FIG. 1: (a) The electron occupation number $< n_i >$ in each quantum dot as a function of the gate voltage ϵ_d. $\Delta\epsilon_d/\Gamma = 0$(solid line); 2.0 (dashed line). The other used parameters are $D = 1.0$, $t_c = 0$, $\Gamma = 0.01$, $U/\Gamma = 10$, and $V = U/2$; (b) The interdot spin correlation $< \mathbf{S}_1 \cdot \mathbf{S}_2 >$ as a function of the gate voltage ϵ_d.

III. RESULTS AND DISCUSSIONS

In the following, we will present the results of our NRG calculation. For the sake of simplicity, we only consider the symmetric coupling case with the hybridization strength $\Gamma_1 = \Gamma_2 \equiv \Gamma$. We take the bandwidth $D = 1$ as the energy unit, and the other parameters $\Gamma = 0.01$, $U = 10\Gamma$, $V = U/2$. One can define the averaged energy level of QDs as $\epsilon_d = (\epsilon_1 + \epsilon_2)/2$, and the energy level difference $\Delta\epsilon_d = \epsilon_2 - \epsilon_1$. Both of them can be tuned experimentally by external gate voltages.

At first, we consider DQDs without interdot tunneling ($t_c = 0$). In Fig.1(a) the occupation number of electrons $< n_i >$ in each QD is plotted as a function of the average energy level ϵ_d. The electron occupation number increases consecutively by tuning the QD level below the Fermi energy. For this DQDs with interdot capacitive interaction, one can easily discern the different regions of occupation states: from empty occupation to the state with total four electrons in DQDs . In the case of two identical QDs ($\Delta\epsilon_d = 0$), abrupt jumps of the occupation number are observed at some particular gate voltage. One can see that the position of jumps can be identified as the region where the DQDS have odd number of electrons. For DQDs with different energy levels($\Delta\epsilon_d \neq 0$), the QD with low energy level is occupied first, and because of interdot capacitive interaction, it will greatly suppress the occupation of electron in another QD as compared with the two identical QDs case. The interdot spin-correlation $< \mathbf{S}_1 \cdot \mathbf{S}_2 >$ as a function of energy level ϵ_d is shown in Fig.1(b), where the spin operators in the i-th QD are defined by $\mathbf{S}_i = 1/2 \sum_{\sigma\sigma'} d^\dagger_{i\sigma}\sigma_{\sigma\sigma'}d_{i\sigma'}$. It shows that the interdot spin correlation is antiferromagnetic in the mixed valence regime, and is ferromagnetic in the doubly occupied regime, where each QD is occupied by one electron. For DQDs with energy level difference, the spin correlation in mixed valence regime is greatly suppressed, but there are still large ferromagnetic spin correlation in the doubly occupied regime. In the identical QDs($\Delta\epsilon_d = 0$) case, the abrupt jumps in occupancy and the spin correlation turn from FM to AFM have also been found in Ref.[23] for N-QD system($N \geq 2$) without interdot capacitive coupling, and this phenomenon is interpreted as a kind of quantum phase transitions. However, one can see from the dashed line in Fig.1 that the abrupt jumps both in occupancy and spin correlation disappear when $\Delta\epsilon_d \neq 0$, hence this kind of phase transition is unstable with respect to the perturbation by gate voltage difference in QDs. We attribute this kind of abrupt jump as a result of Fano resonance and the crossing of the antibonding state energy level with the Fermi energy.

Next, we calculate the electron conductance through DQDs when a small bias voltage is applied to the leads. In Fig.2 the linear conductance G at zero temperature vs. the average QD energy level ϵ_d is depicted. As shown in Fig.2(a), the Kondo effects are manifested by peaks in the curve of the linear conductance, where the conductances approach the unitary limit ($G = 2e^2/h$). In the regime of odd electron occupation, the DQDs act as a localized spin (s=1/2), and the Kondo effect is arose from the spin exchange interaction between the localized electron spin and that of the electrons in the leads. Whereas, in the doubly occupied regime, the unitary conductance is due to the underscreened spin 1 Kondo effect, It will be shown in the following that in this regime the two electrons confined in the DQDS form a spin triplet state in the ground state. In the presence of sufficient interdot tunneling t_c, the Kondo effect in the singly occupied regime and spin 1 Kondo effect is strongly suppressed, but some asymmetrical peaks of conductance appears in the mixed valence regime, this can be attributed to the Fano resonance for the electron transport through the bonding and antibonding channels in this system. It is interesting to notice that in the triply occupied regime the conductance still achieves the unitary limit even in the presence of strong interdot tunnel coupling.

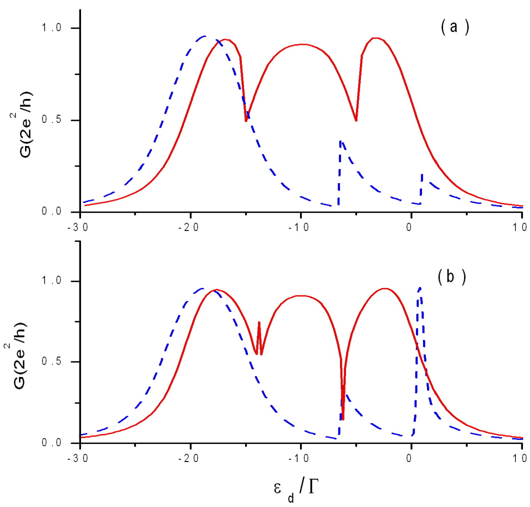

FIG. 2: The linear conductance G as a function of the dot level at zero temperature. (a) for the system with two identical quantum dots($\Delta\epsilon_d = 0$); (b) for DQDs with energy level difference($\Delta\epsilon_d/\Gamma = 2.0$). The interdot tunneling parameter takes $t_c/\Gamma = 0$(solid line) and $t_c/\Gamma = 2.0$(dashed line), respectively.

In the following, we will focus our attentions on the properties in the doubly occupied regime. In order to illustrate the effect of interdot tunneling, the transmission probability at different tunneling coupling t_c is shown in Fig.3 (a). Without direct interdot tunneling ($t_c = 0$), one can see that the transmission probability has the particle-hole symmetry, and the spin exchange effect between the electrons localized in the quantum dots and that in the leads gives rise to a sharp peak in the transmission probability at the Fermi surface, therefore the linear conductance at zero temperature reaches the unitary limit $G = 2e^2/h$, as a result of the underscreened

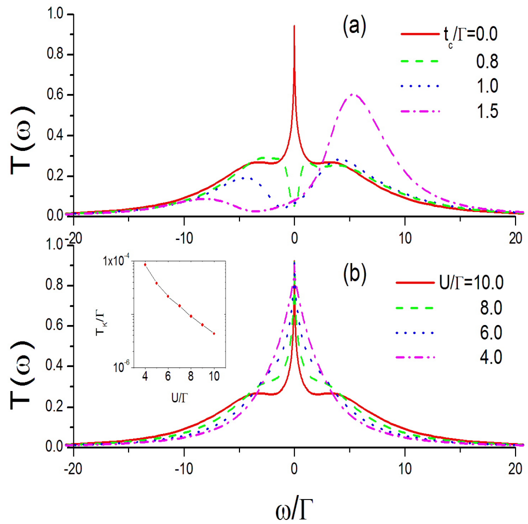

FIG. 3: (a) The transmission probability $T(\omega)$ for the system with two identical quantum dots. Used parameters are $D = 1.0$, $\Gamma = 0.01$, $U/\Gamma = 10$, $V = U/2$ and $\epsilon_d/\Gamma = -10.0$. The interdot tunnel coupling $t_c/\Gamma = 0.0, 0.8, 1.0, 1.5$, respectively. (b) The transmission probability $T(\omega)$ at the particle-hole symmetric point for different values of on-site Coulomb interaction U. Inset: the estimated Kondo temperature T_K vs. the value of U.

spin 1 Kondo effect. In the presence of the interdot coupling $t_c \neq 0$, the particle-hole symmetry of the transmission probability is broken. When t_c increases beyond a quantum critical point, a sharp dip in the transmission probability is observed. It suggests that the Kondo effect and the linear conductance in this regime is strongly suppressed. Therefore, there is a quantum phase transition between underscreened Kondo phase and the local spin singlet phase in the ground state of this system. For two-impurity Anderson model without interdot capacitive coupling, this quantum phase transition has been predicted by Nishimoto et al. by using dynamic density matrix renormalization group [25], and Žitko et al. have obtained its thermodynamic properties, such as the temperature dependence of magnetic susceptibility and entropy by NRG method [26]. It is noted that a similar quantum phase transition is also observed in two-level single QD system with intradot spin exchange coupling by Hund's rule[19]. For DQDs with RKKY interaction coupled to two-channel lead, Chung et al.[20] found the quantum phase transition is from Kondo screened phase to spin singlet phase. In Fig.3(a), by further increasing the interdot coupling t_c, a broad peak of transmission probability with the line shape of Breit-Wigner resonance is developed around the energy $\omega \approx U/2$, we attribute this broad transmission peak to the electron transport through the bonding channel of electrons in the quantum dots.

In Fig.3(b) the transmission probability $T(\omega)$ at different values of on-site Coulomb interaction U is depicted. It shows that the line shape of the $T(\omega)$ changes significantly by varying the Coulomb interaction strength U. The line shape becomes more cusplike with decreasing U , and it reveals that the physical properties of this underscreened Kondo effect in DQD system is quite different from the spin 1/2 Kondo effect. For the spin 1/2 Kondo effect in single-impurity Anderson model, one can estimate the Kondo temperature T_K by using the formula $T_K = \frac{\sqrt{U\Gamma}}{2} exp[\epsilon_d(\epsilon_d + U)/U\Gamma]$. For this underscreened Kondo effect case, we make the following approximation to estimate the Kondo temperature : at the frequency of $\omega = T_K$ the transmission probability $T(\omega = T_K)/T(\omega = 0) \approx 0.978$. For the single-impurity Anderson model, T_K obtained by this approximation agrees well with the above formula. The inset of Fig.3 (b) shows the estimated T_K at several values of the Coulomb interaction strength U for the DQD system. For the system with the parameters used in our calculation, the Kondo temperature T_K is on the order of $10^{-5}\Gamma$.

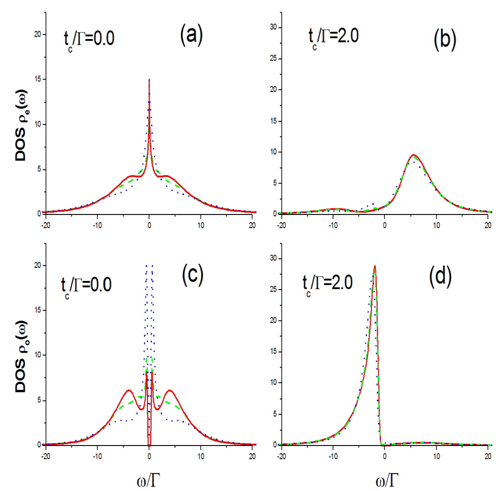

FIG. 4: The density of state of the local bonding and antibonding states in the quantum dot at different values of energy level difference: $\Delta\epsilon_d/\Gamma = 0.0$(solid line), 2.0(dashed line), 4.0(dotted line). (a), (b) corresponds to the bonding state with $t_c/\Gamma = 0, 0, 2.0$, respectively. (c),(d) are that of the antibonding states. The other used parameters are the same as in Fig.3.

In order to get better understanding of the electron state in the system, we investigate the local density of states(DOS) in the DQDs. One can define the even orbital (bonding state) operator as $d_{e,\sigma} = (d_{1\sigma} + d_{2\sigma})/\sqrt{2}$, and the odd orbital (antibonding state) operator $d_{e,\sigma} = (d_{1\sigma} - d_{2\sigma})/\sqrt{2}$. The local density of state for the bonding and antibonding states are depicted in Fig.4. As shown in Fig.4(a) and (c), in the absence of interdot coupling($t_c = 0$), the local DOS of even and odd orbital

retain the particle-hole symmetry of the system. It is noticed that the transmission probability is proportional to the DOS for the bonding state, therefore a Kondo peak around the Fermi energy is observed in its DOS. Some new features are also manifested in DOS for this system, one can see that the DOS for the antibonding state has two side peaks nearby the Fermi energy , which can be understood as a result of the effective spin-exchange interaction between the electrons in DQDs by tunneling through the leads, and this feature cannot be found in DQDs in serial configuration[18]. As the interdot coupling t_c is large than some critical value(see Fig. 4(b) and (d)), the Kondo effect on the DOS of bonding state is greatly suppressed, and a broad peak around the energy $\omega \approx U/2$ are developed. For the DOS of the antibonding state, a sharp peak is developed slight below the Fermi energy, this is due to the fact that the antibonding state of electrons in DQDs seems like a quasi-localized state. Increasing the interdot coupling t_c further, the sharp peak is broaden and shifts away from the Fermi surface to lower energy. For DQDs with different energy levels, the characteristic features of the DOS remain unchanged.

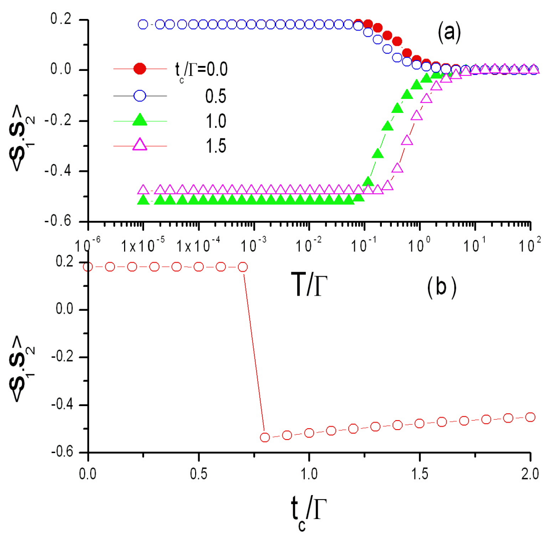

FIG. 5: (a)The spin correlation $< \mathbf{S}_1 \cdot \mathbf{S}_2 >$ of double quantum dots as a function of temperature T for several different values of t_c. (b) The spin correlation $< \mathbf{S}_1 \cdot \mathbf{S}_2 >$ vs. the interdot tunnel coupling t_c at zero temperature. The other used parameters are the same as in Fig.3.

To gain more insight into the spin entanglement and the effect of spin exchange interaction for the electrons localized in different QDs, We have also calculated the interdot spin-correlation $< \mathbf{S}_1 \cdot \mathbf{S}_2 >$ as a function of temperature for several values of interdot tunneling t_c as shown in Fig.5(a). When interdot tunneling t_c is zero or has a small value, one can see that the spin-correlation converges to a positive value as temperature decreases. It is easy to notice that the positive value of $< \mathbf{S}_1 \cdot \mathbf{S}_2 >$ reveals that the spin-correlation in this case is ferromagnetic type in the ground state. As we know that when two ideal spin $s = 1/2$ electrons form a spin triplet, the spin-correlation will be $< \mathbf{S}_1 \cdot \mathbf{S}_2 >= 1/4$. The rather high positive value of spin-correlation indicates that electrons localized in QDs still have high probability to form a spin triplet even though they are coupled with the electrons in the leads in the Kondo regime. By increasing the interdot coupling t_c, there exhibits a quantum phase transition from the triplet state to singlet state in the ground state. The spin correlation approach a negative value $< \mathbf{S}_1 \cdot \mathbf{S}_2 > \approx -0.50$, as we know that for two electrons forming an ideal spin singlet$< \mathbf{S}_1 \cdot \mathbf{S}_2 >= -0.75$, therefore the electrons in DQDs is largely in a singlet state. In order to determine the critical value of t_c, we have calculated the spin correlation $< \mathbf{S}_1 \cdot \mathbf{S}_2 >$ at zero temperature for different value of t_c, the result is shown in Fig.5(b). We find that, at the quantum critical point $t_c \approx 0.7$, there is an abrupt jump of the spin correlation $< \mathbf{S}_1 \cdot \mathbf{S}_2 >$. It indicates that the quantum phase transition from triplet to singlet state is of first order kind. According to a previous study on two-impurity Kondo model[27], we may expect that in the case of DQDs with energy level difference, this kind of first order transition will become Kosterlitz-Thouless type. It is easy to understand that the exact quantum critical value of t_c will depends on the the interaction parameters, such as the onsite Coulomb repulsion U, interdot capacitive coupling V and the energy level ϵ_d, etc.

IV. SUMMARY

In summary, we have studied the ground state and the electron transport properties of the system with DQDs in parallel configuration. The strong on-site Coulomb repulsion and the interdot capacitive coupling is taken into account by the nonperturbative NRG technique. It is shown that the large interdot tunneling will drastically change the transport properties in this system. The ground state of DQDs exhibits a quantum phase transition from triplet state to singlet state by increasing the interdot tunneling amplitude. In the case of no interdot tunneling, the linear conductance approaches to unitary limit in the doubly occupied regime due to the underscreened Kondo effect, whereas it is greatly suppressed when the electrons in DQDs form an singlet state with the interdot coupling t_c being larger than the critical value. For the DQDs with strong interdot tunneling, the Fano resonance can be observed in the linear conductance when the system are in the mixed valence regime. One may expect that the underscreened Kondo effect can be observed in future experiments on DQD system without direct interdot tunneling.

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